3. Solving Parabolic PDEs with R

Modeling with PDEs

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Elliptic, Parabolic, and Hyperbolic Equations

- The general form of a linear second-order PDE in two dimensions is:

$$A \cdot u_{xx} + B \cdot u_{xy} + C \cdot u_{yy} + D \cdot u_x + E \cdot u_y + F = 0$$

- Depending on the sign of the *discriminant*

$$d = A \cdot C - B^2$$

linear second-order PDEs are called:

  - *elliptic* if $d > 0$
  - *parabolic* if $d = 0$
  - *hyperbolic* if $d < 0$

Examples of Parabolic Equations

- Heat equation:

$$\frac{\partial T}{\partial t} - \frac{K}{C\rho}\left(\frac{\partial^2 T}{\partial x^2}\right) = 0$$

$$-\frac{K}{C\rho}\frac{\partial^2 T}{\partial x^2} + 0\frac{\partial^2 T}{\partial x \partial t} + 0\frac{\partial^2 T}{\partial t^2} + 0\frac{\partial T}{\partial x} + \frac{\partial T}{\partial t} + 0 = 0$$

$$A = -\frac{K}{C\rho} \quad B = 0 \quad C = 0 \quad D = 0 \quad E = 1 \quad F = 0$$

$$d = A \cdot C - B^2 = 0 \Rightarrow Parabolic$$

Examples of Parabolic Equations

- Action potential propagation in a fiber:

$$C_m \frac{\partial V_m}{\partial t} - \sigma \frac{\partial^2 V_m}{\partial x^2} + I_{ion} = 0$$

$$-\sigma \frac{\partial^2 V_m}{\partial x^2} + 0 \frac{\partial^2 V_m}{\partial x \partial t} + 0 \frac{\partial^2 V_m}{\partial t^2} + 0 \frac{\partial V_m}{\partial x} + C_m \frac{\partial V_m}{\partial t} + I_{ion} = 0$$

$$A = -\sigma \quad B = 0 \quad C = 0 \quad D = 0 \quad E = C_m \quad F = I_{ion}$$

$$d = A \cdot C - B^2 = 0 \Rightarrow Parabolic$$

Re-Cap of the Classification

- **Elliptic PDEs:** Contains second-order derivatives with respect to all independent variables, which all have the same sign.
- **Parabolic PDEs:** Involve one second-order derivative and at least one first-order derivative.
- **Hyperbolic PDEs:** Similar to Elliptic but the second-order derivatives have switching signs.

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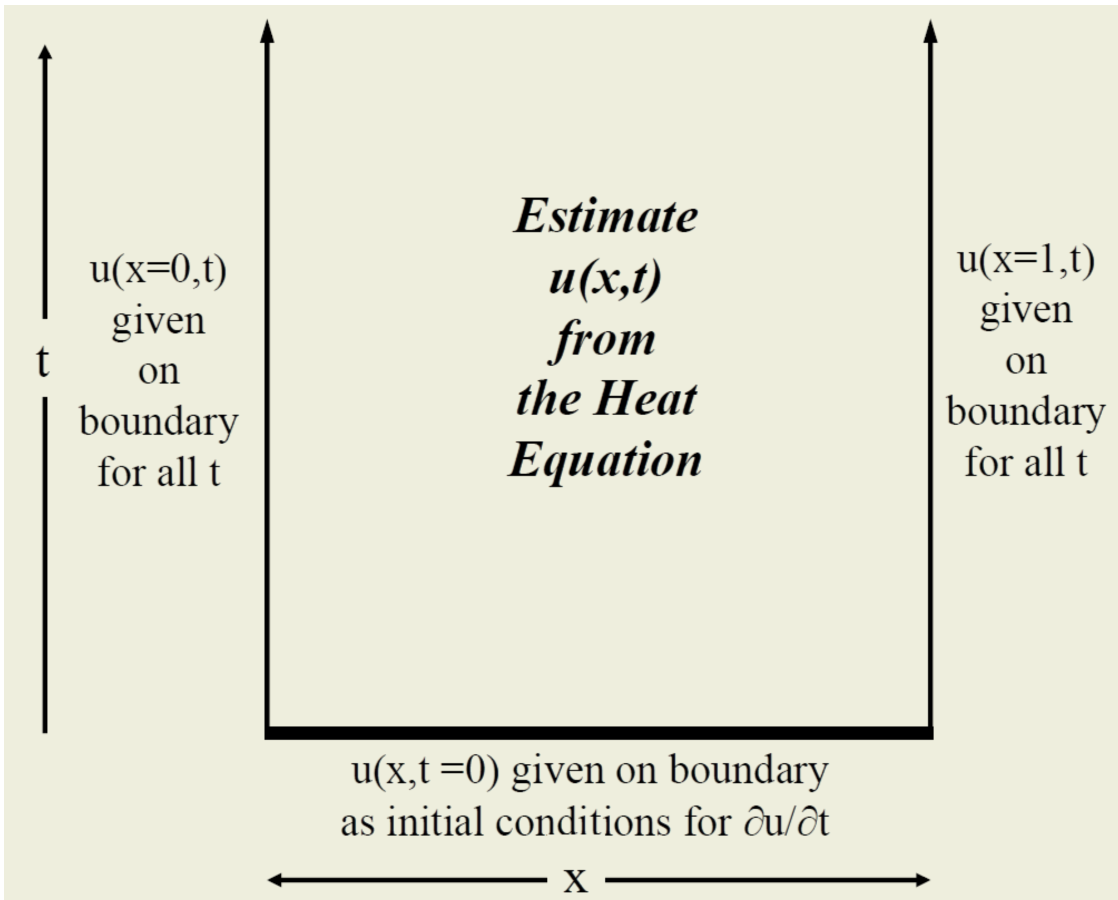
Parabolic PDE's

- Typically provided are
  - Initial values: $u(x, t = 0)$
  - Boundary conditions: $u(x = x_0, t)$ for all t

- All changes are propagated forward in time, i.e., nothing goes backward in time; changes are propagated across space at decreasing amplitude

Parabolic PDE's



Numerical Methods for Solving PDEs

- The numerical methods used for solving PDE's are different depending on the different character of the problems.
  - Sometimes, the problem is solved at all the positions once for steady state conditions
  - Other times, we need to integrate using the initial conditions forward through time.

Numerical Methods for Solving PDEs

- **Methods**

  - **Finite Difference Method (FDM):** Based on approximating solution at a finite # of points, usually arranged in a regular grid.

  - **Finite Element Method (FEM):** Based on approximating solution on an assemblage of simply shaped (triangular, quadrilateral) finite pieces or "elements".

  - **Method of Lines**: valid for PDEs that are formulated as an initial-value problem in one of its variables. Based on a reformulation of the PDE in terms of a system of ODEs or differential-algebraic equations.

Finite Difference Method

- Based on approximating solution at a finite # of points, usually arranged in a regular grid.

- Similar to the Forward Euler integration: derivatives are approximated using the difference between two points with an small separation

Solving Parabollic PDE’s

- **Solution of Parabolic PDE's by FD Method**
  1. Discretize the domain into a grid of evenly spaces points (nodes)
  2. Express the derivatives in terms of Finite Difference

$$\frac{\partial^2 T}{\partial x^2} \quad \frac{\partial T}{\partial t} \rightarrow Fitine\ differences$$

  3. Choose Δx and Δt and use the initial values and the boundary conditions to solve the problem by systematically moving ahead in time.

Solving Parabollic PDE’s

- Time derivative:
  - **Explicit:** The future value $(t + \Delta \mathrm{t})$ are calculated using the actual values (t) and the previous values $(\mathrm{t} - \Delta \mathrm{t})$
  - **Implicit:** The future values $(t + \Delta \mathrm{t})$ are calculated using the actual values (t), the future values $(t + \Delta \mathrm{t})$, and, sometimes, the previous values $(t - \Delta \mathrm{t})$

Example: Explicit 1D-Heat equation

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2}$$

- **Notation:** Subscripts (i) for space and subscripts (m) for time.
- The ecuation can be aproximated by:

$$\frac{\partial T}{\partial t} \approx \frac{T_{i,m+1} - T_{i,m}}{\Delta t}$$

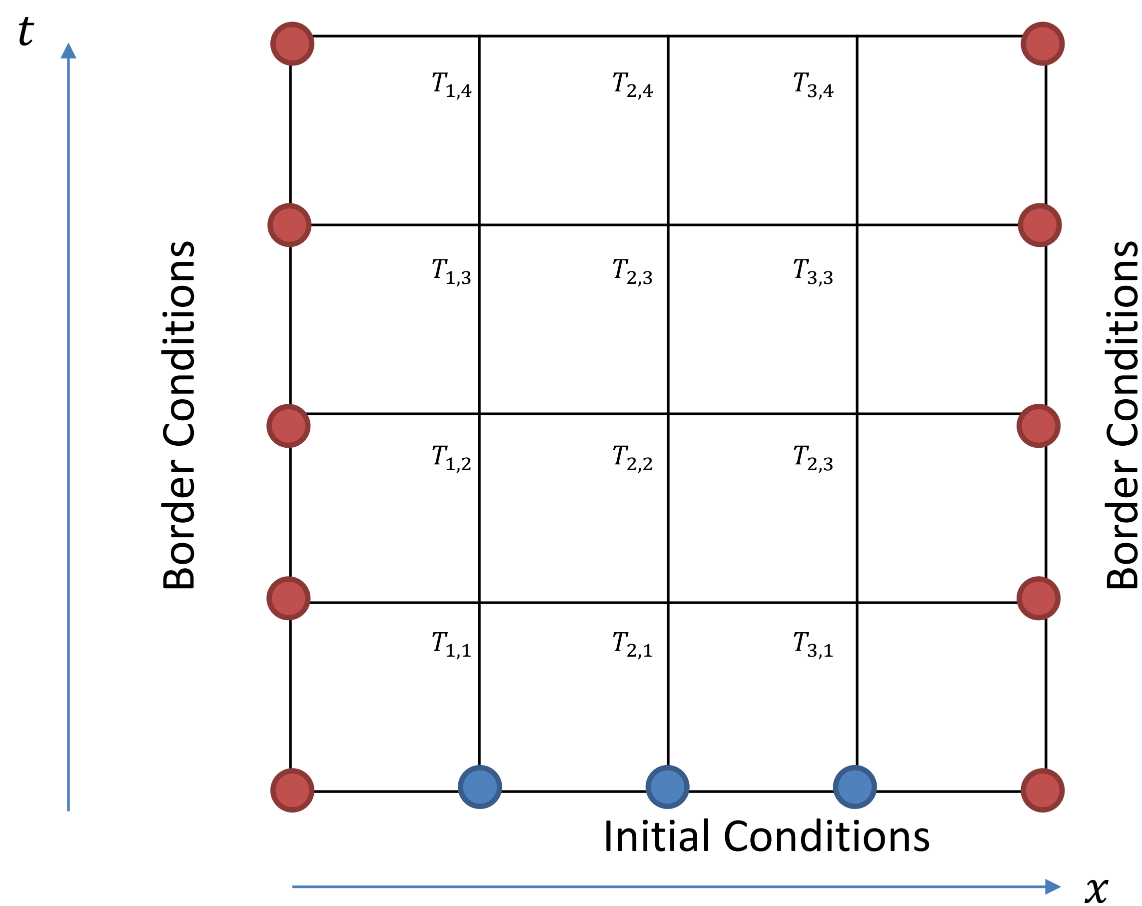
$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i-1,m} - 2T_{i,m} + T_{i+1,m}}{\Delta x^2}$$

$$\frac{T_{i,m+1} - T_{i,m}}{\Delta t} \approx \frac{K}{C\rho} \frac{T_{i-1,m} - 2T_{i,m} + T_{i+1,m}}{\Delta x^2} \Rightarrow$$

$$\Rightarrow T_{i,m+1} \approx T_{i,m} + \frac{\Delta t}{\Delta x^2} \frac{K}{C\rho} \left(T_{i-1,m} - 2T_{i,m} + T_{i+1,m} \right)$$

Example: Explicit 1D-Heat equation

$$T_{i,m+1} \approx T_{i,m} + \frac{\Delta t}{\Delta x^2}\frac{K}{C\rho}\left(T_{i-1,m} - 2T_{i,m} + T_{i+1,m}\right)$$



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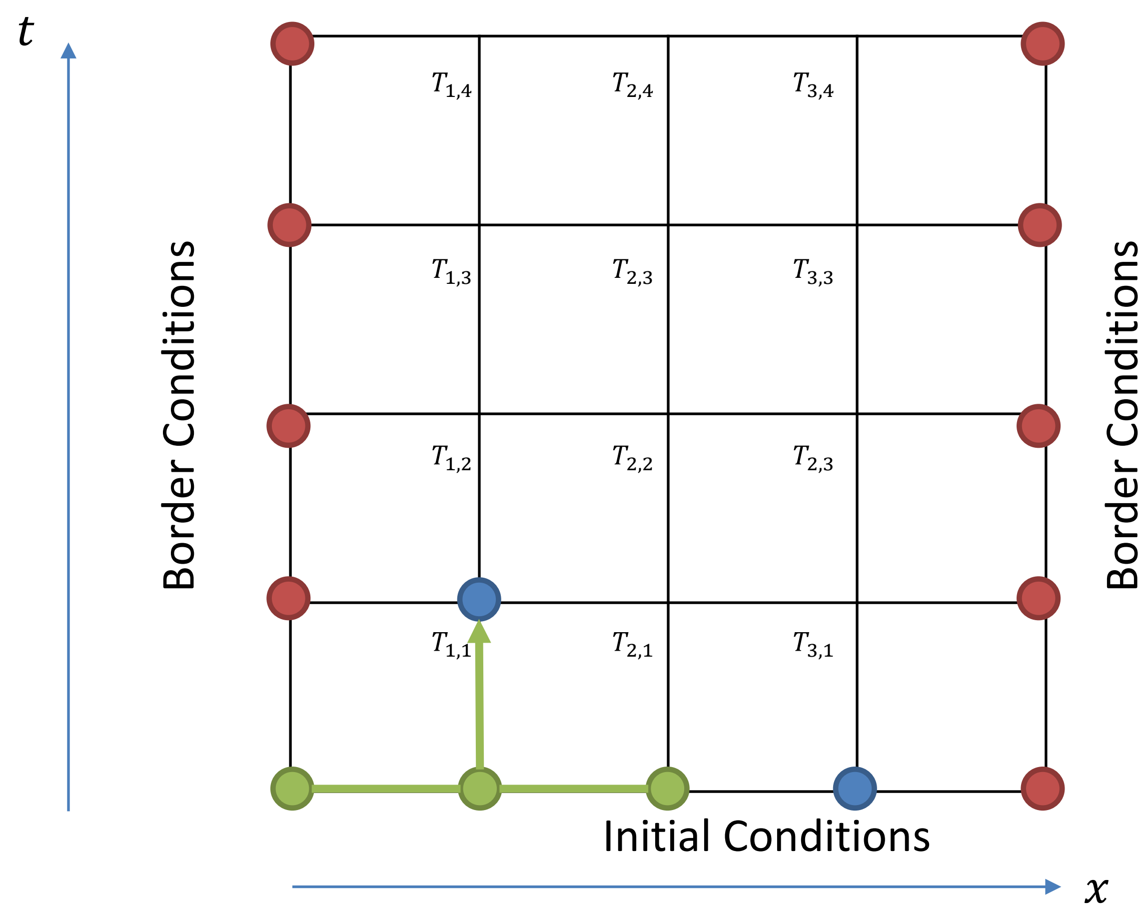

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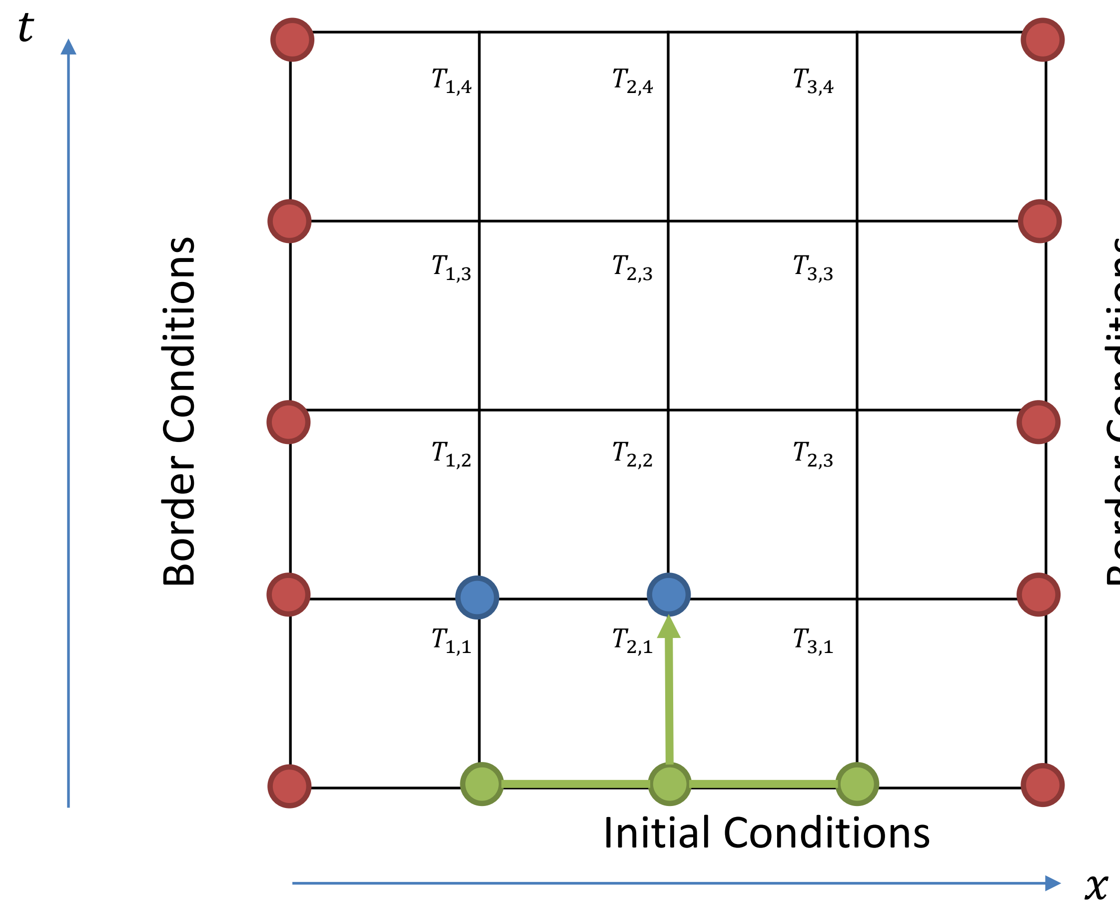

Example: Explicit 1D-Heat equation

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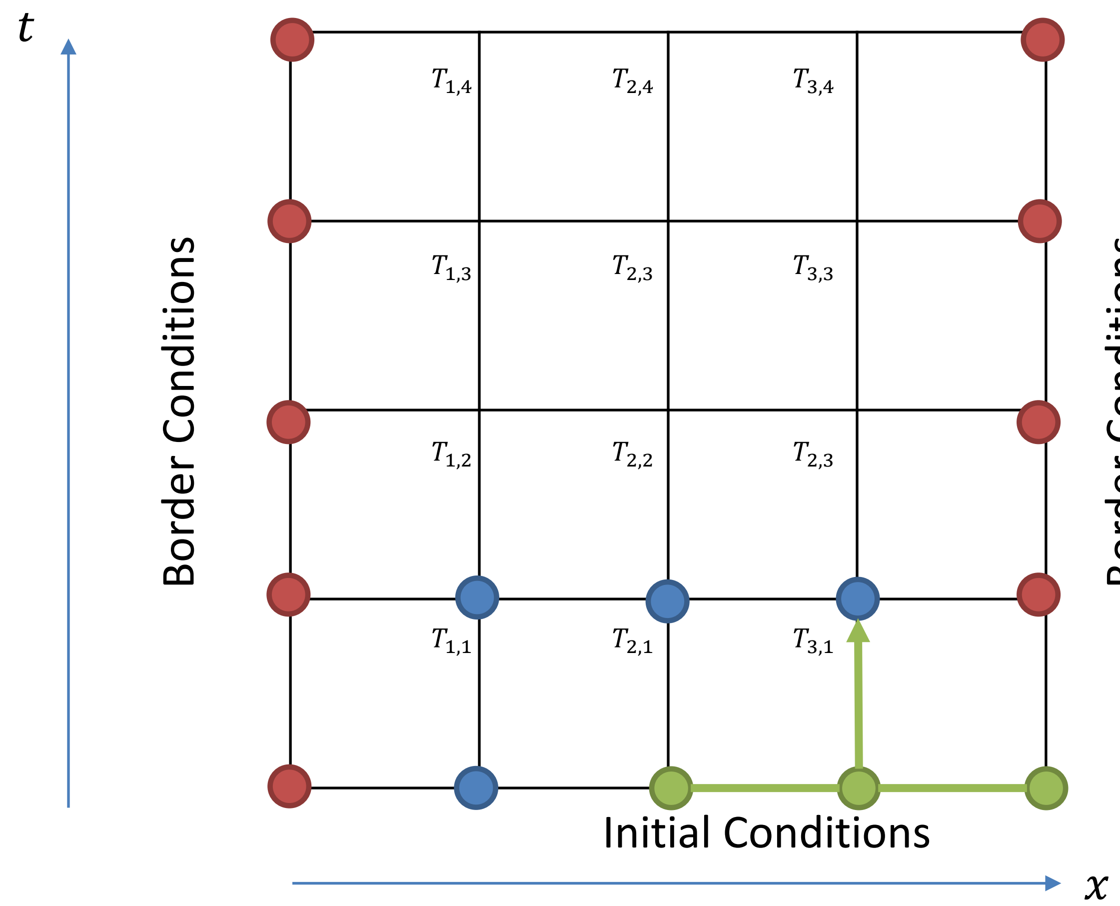
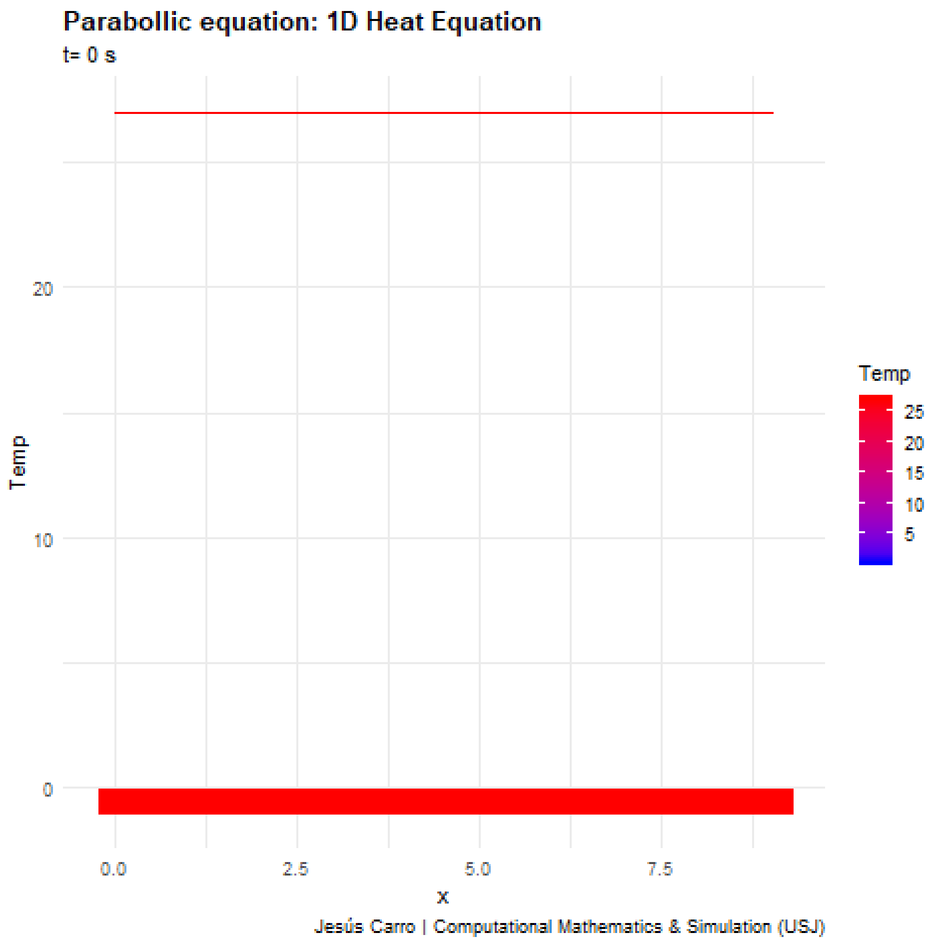


Example: Explicit 1D-Heat equation



Example: Explicit 1D-Heat equation

- Libraries:
  - gganimate
  - transformr
  - gifski
  - png
- Code:

```
anim <- p + transition_time(time) +
  labs(title= 't= {frame_time} s’)

animate(anim,
        nframes = ...,
        start_pause = ...,
        end_pause = ...,
        duration = ...,
        renderer = gifski_renderer(“name.gif"))
```

Example: Explicit 1D-Heat equation

- **Stability:**
  - The Explicit method is conditionally stable
  - For the 1-D spatial problem, the following is the stability condition:

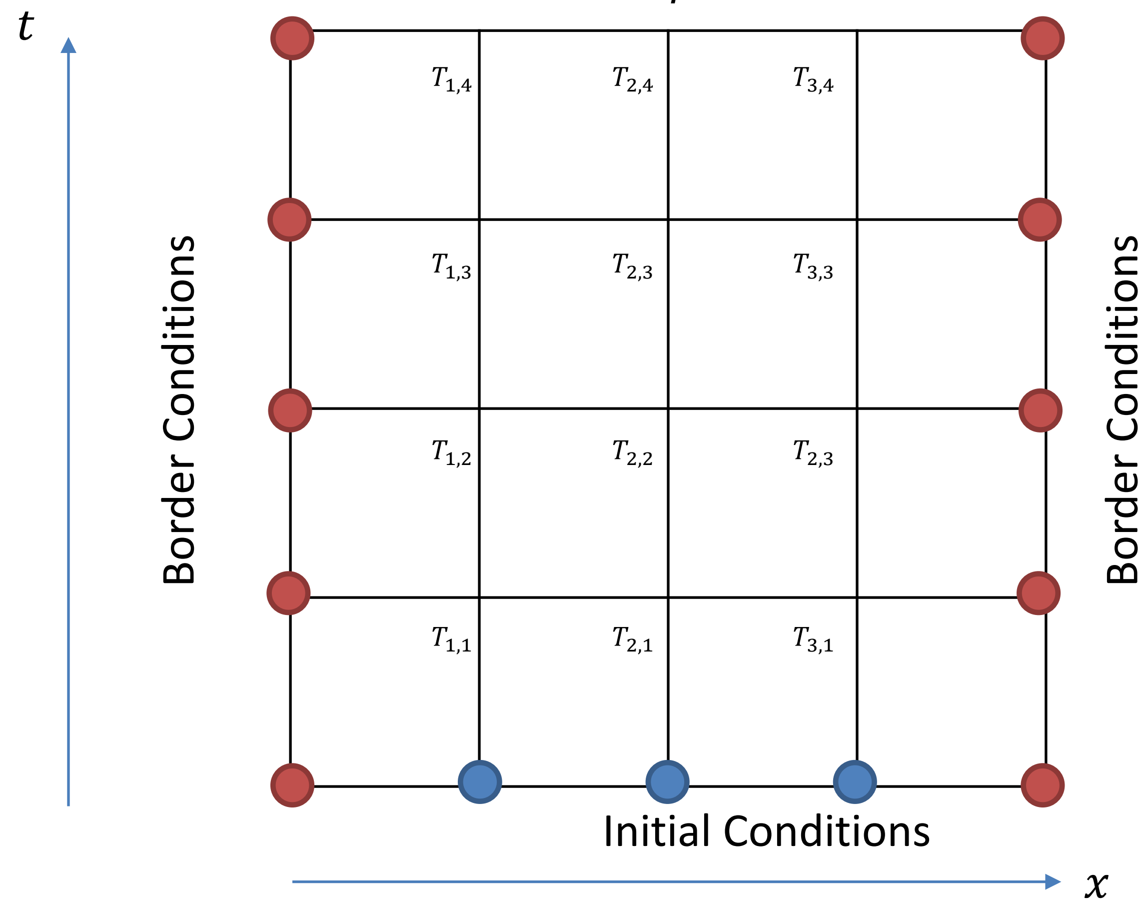
$$\lambda = \frac{\Delta t}{\Delta x^2}\frac{K}{C\rho}$$

    - $\lambda \leq \frac{1}{2}$ can still yield oscillation (1D)
    - $\lambda \leq \frac{1}{4}$ ensures no oscillation (1D)
    - $\lambda \leq \frac{1}{6}$ tends to optimize truncation error

  - Implicit Methods are unconditionally stable.

Exercise: Implicit 1D-Heat equation

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2}$$



Exercise: Implicit 1D-Heat equation

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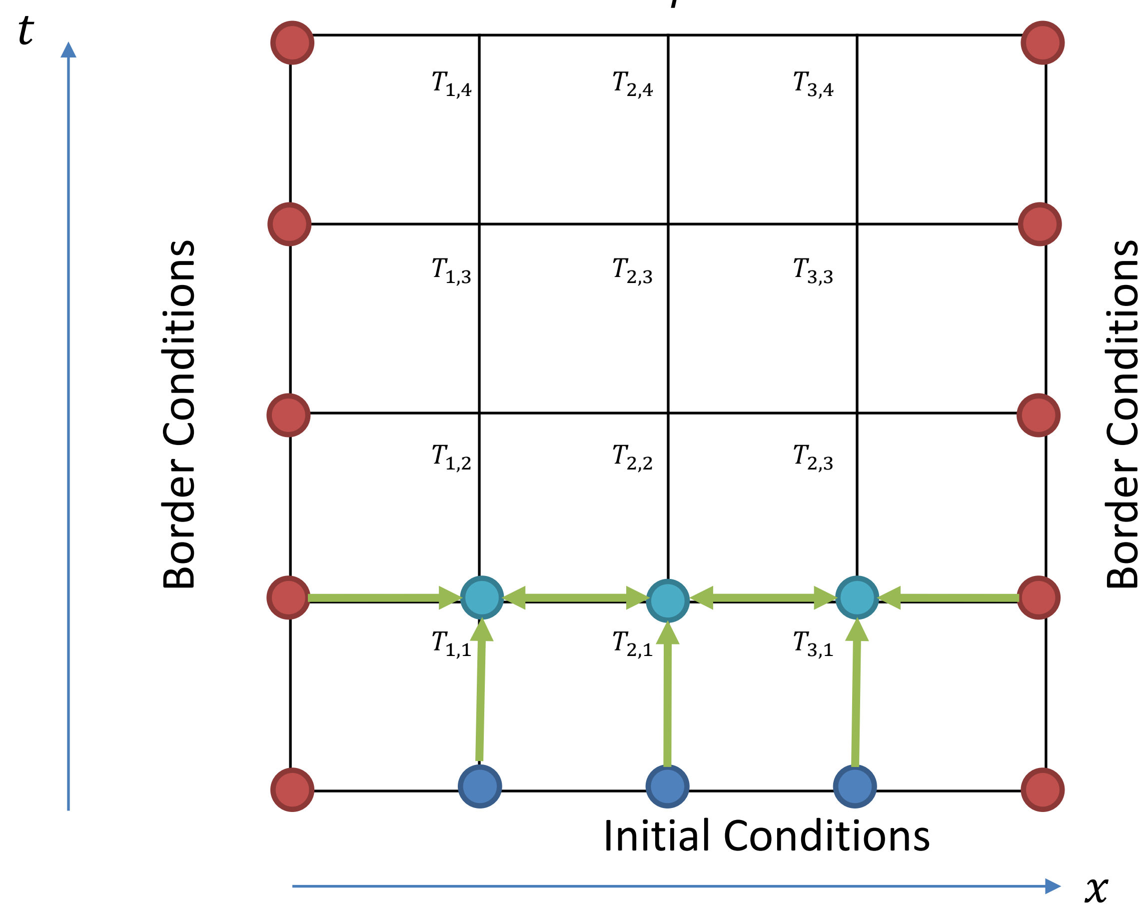

Exercise: Implicit 1D-Heat equation

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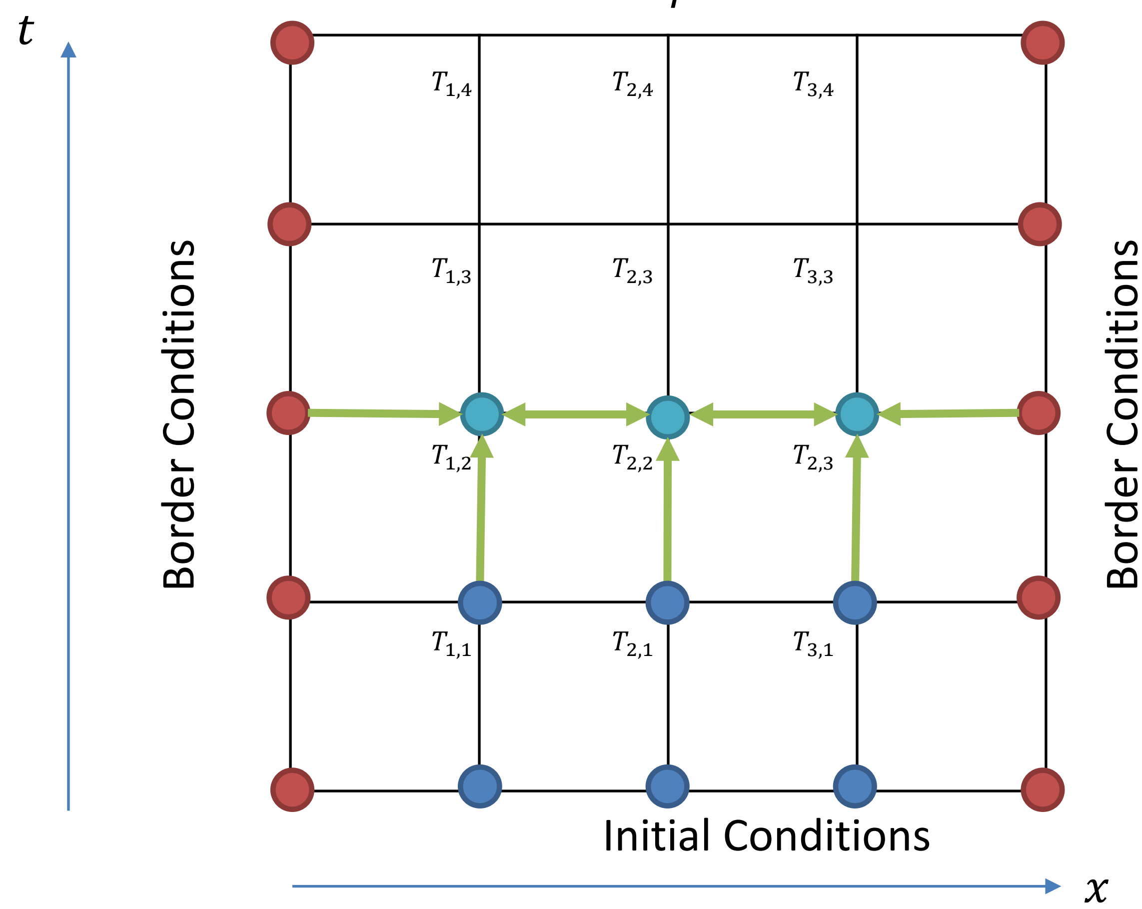

Exercise: Implicit 1D-Heat equation

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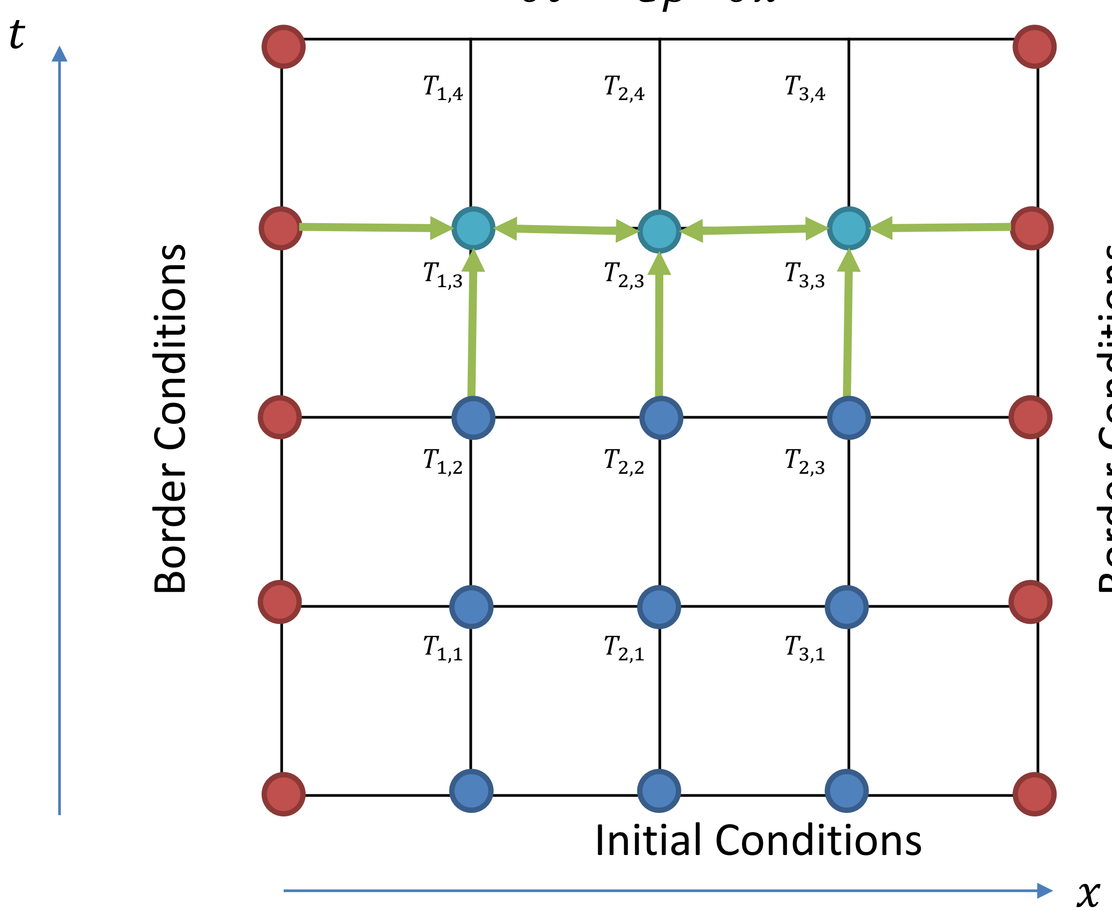


Solution: Implicit 1D-Heat equation

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2}$$

- The ecuation can be aproximated by:

$$\frac{\partial T}{\partial t} \approx \frac{T_{i,m+1} - T_{i,m}}{\Delta t}$$

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i-1,m+1} - 2T_{i,m+1} + T_{i+1,m+1}}{\Delta x^2}$$

$$\lambda = \frac{\Delta t}{\Delta x^2} \frac{K}{C\rho}$$

$$\frac{T_{i,m+1} - T_{i,m}}{\Delta t} \approx \frac{K}{C\rho} \frac{T_{i-1,m+1} - 2T_{i,m+1} + T_{i+1,m+1}}{\Delta x^2} \Rightarrow$$

$$\Rightarrow T_{i,m+1} - T_{i,m} \approx \lambda\left(T_{i-1,m+1} - 2T_{i,m+1} + T_{i+1,m+1}\right) \Rightarrow$$

$$\Rightarrow T_{i,m} \approx -\lambda \cdot T_{i-1,m+1} + (1 + 2\lambda)T_{i,m+1} - \lambda \cdot T_{i+1,m+1}$$

Solution: Implicit 1D-Heat equation

- In each point a equation can be obtained:

$$T_{i,m} \approx -\lambda \cdot T_{i-1,m+1} + (1+2\lambda)T_{i,m+1} - \lambda \cdot T_{i+1,m+1}$$

- It is necessary to solve a system of equation for all the positions in each interval t.

Solving PDEs in R

- It is necessary to transform the system of PDEs in a system of ODEs

- They can be transformed by numerical differencing.

- Example:

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2} \Rightarrow \frac{\partial T_i}{\partial t} = \frac{K}{C\rho} \cdot \frac{T_{i+1} + T_{i-1} - 2 \cdot T_i}{\Delta x^2}, \qquad i = \{1,2,\dots,n\}$$

  A system with only one state variable is transformed into a system with n state variables

- See the functions `deSolve::ode.1d`, `deSolve::ode.2d`

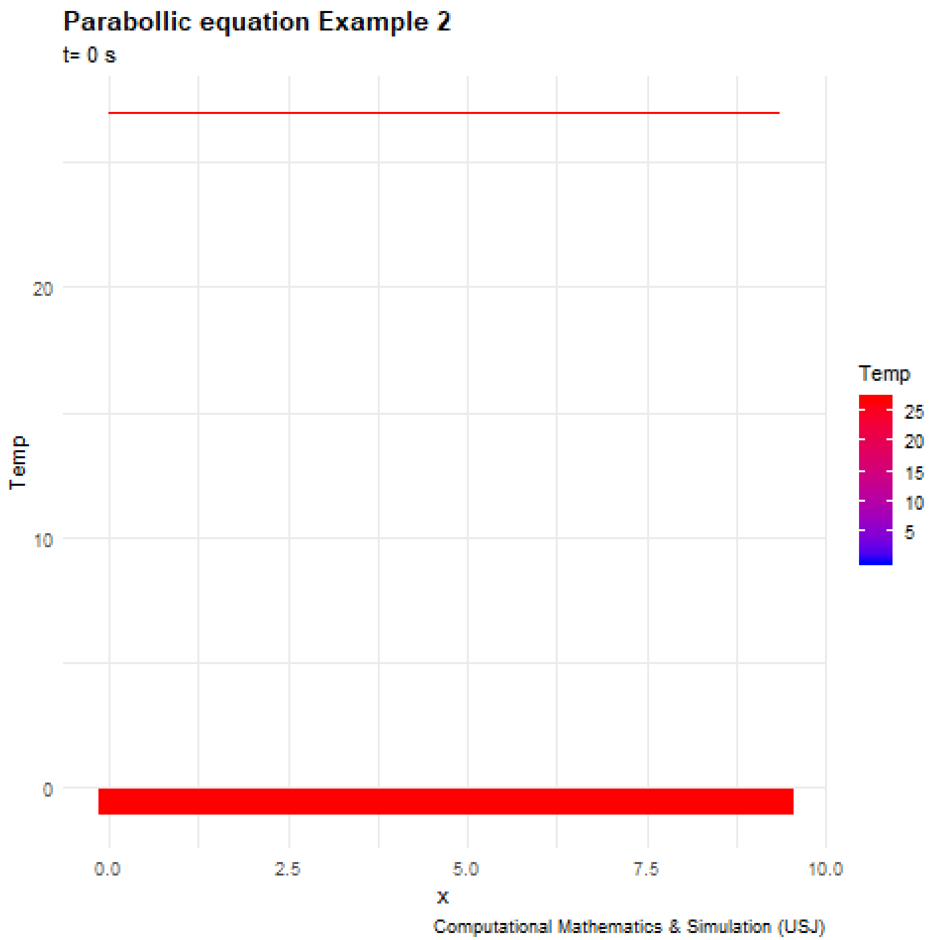
PDE with more terms

- An elliptic or a parabollic equation could have more terms

- Example

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2} - T \cdot e^{-t}$$

PDE with more terms



Operator splitting

- When a PDE or system of PDEs contains different terms expressing different physics
- It is natural to use different numerical methods for different physical processes.
- This is a way to simplify the overall solution process.
- In the context of nonlinear differential equations, operator splitting can be used to isolate nonlinear terms and simplify the solution methods.

Operator splitting

- Example:

$$C_m \frac{\partial V_m}{\partial t} - \sigma \frac{\partial^2 V_m}{\partial x^2} + I_{ion} = 0$$

  - You can integrate the last part for each cell, and with the result we have a simple equation to calculate V_m

Operator splitting Example

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2} - r$$

$$r_{ss} = \frac{10}{1 + T}$$

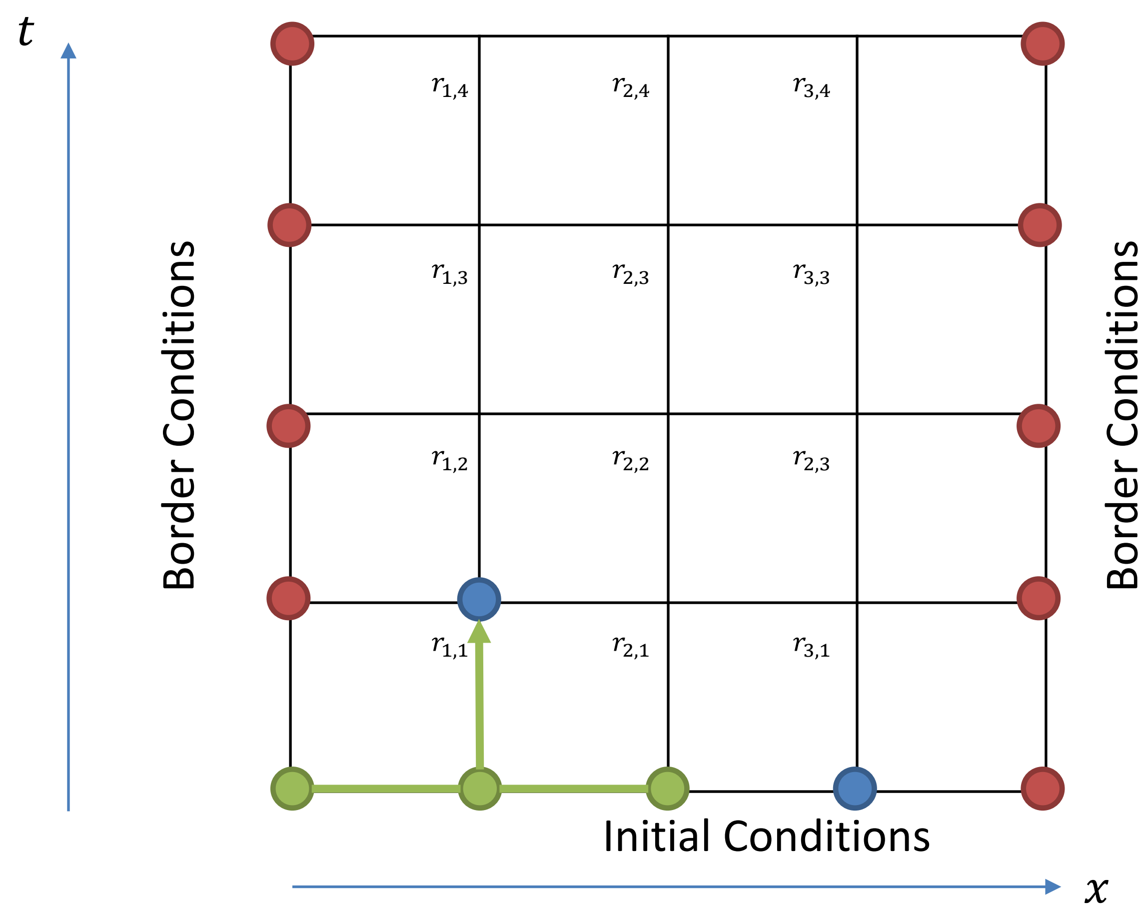
$$\tau_r = 10$$

$$\frac{\partial r}{\partial t} = \frac{r_{ss} - r}{\tau_r}$$

Operator splitting Example

First part: Explicit solver for r

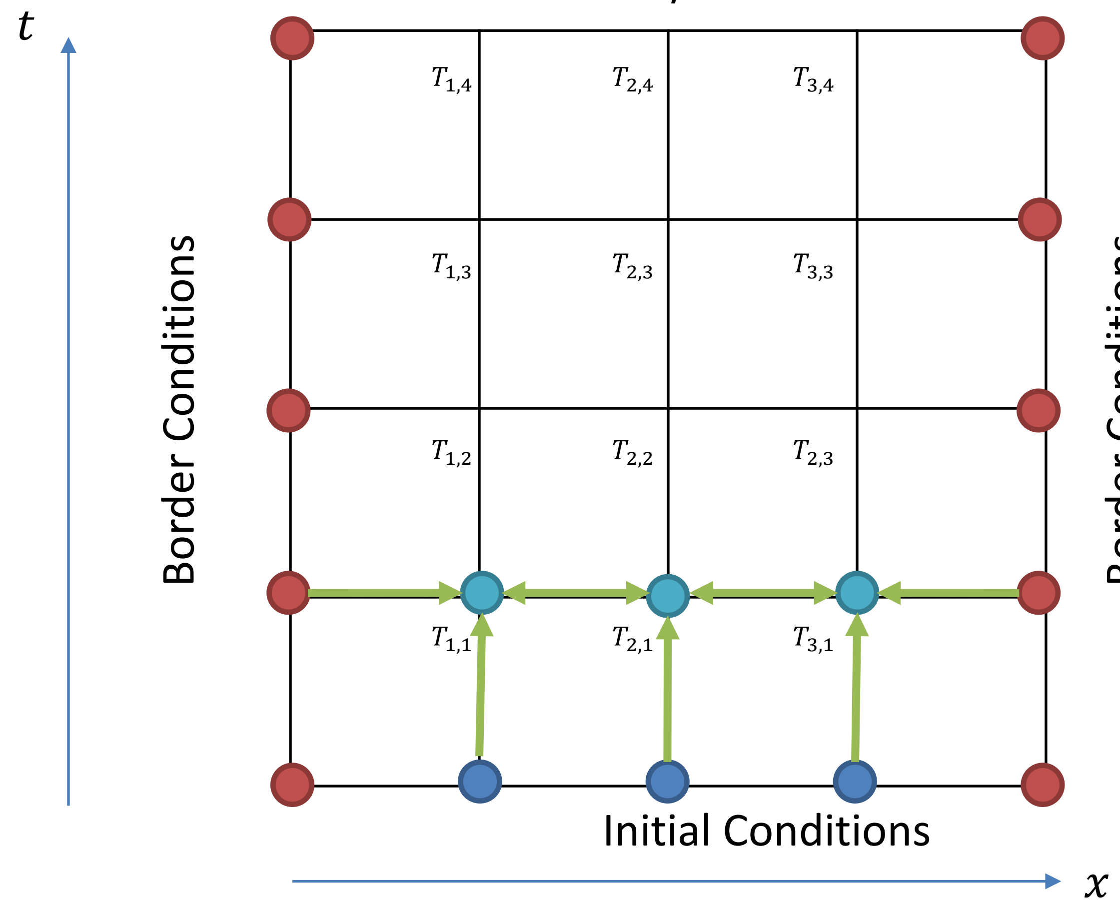
$$r_{i,m+1} \approx r_{i,m} + \Delta t \cdot \frac{\partial r}{\partial t} = r_{i,m} + \Delta t \cdot \frac{r_{ss} - r}{\tau_r}$$



Operator splitting Example

Second part: Implicit solver for T

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2} - r$$



Operator splitting Example

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho} \cdot \frac{\partial^2 T}{\partial x^2} - r$$

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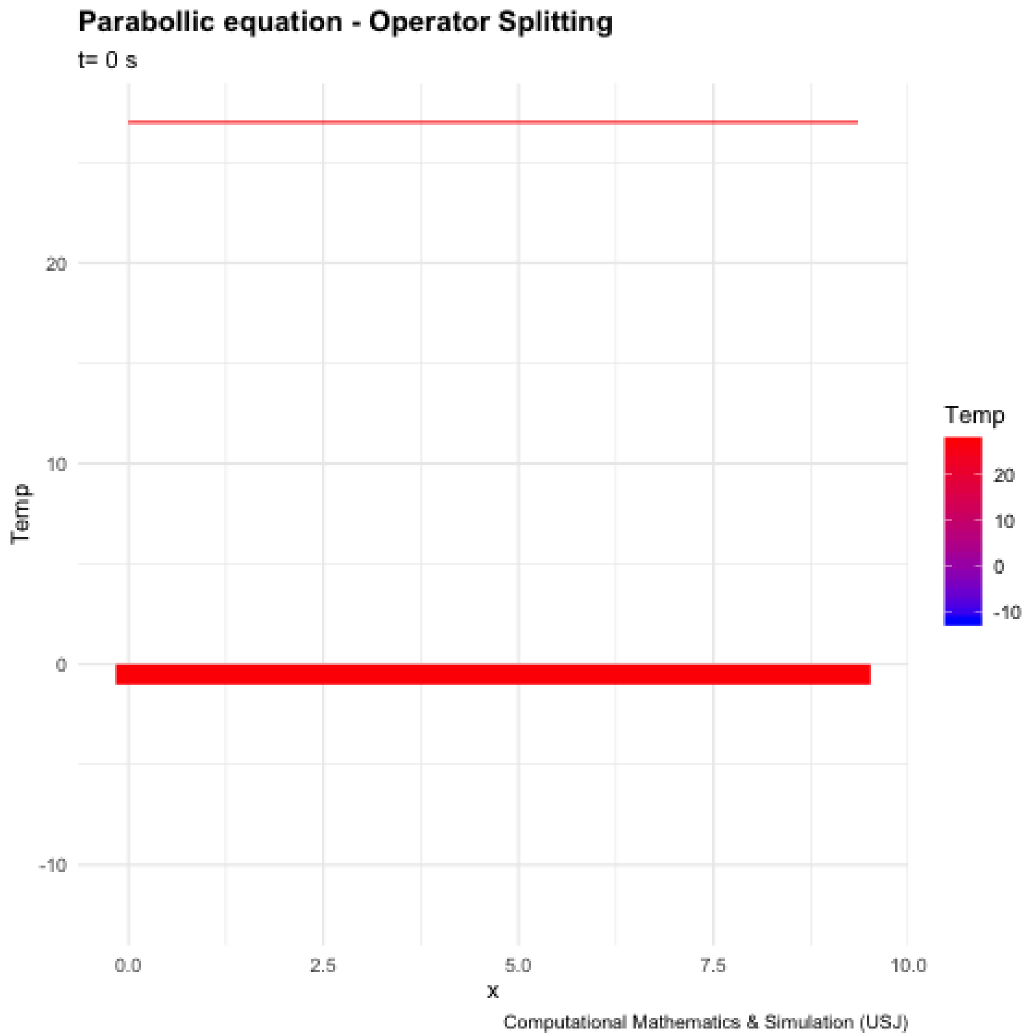
$$\lambda = \frac{\Delta t}{\Delta x^2}\frac{K}{C\rho}$$

$$\frac{T_{i,m+1} - T_{i,m}}{\Delta t} \approx \frac{K}{C\rho}\frac{T_{i-1,m+1} - 2T_{i,m+1} + T_{i+1,m+1}}{\Delta x^2} - r_{i,m+1} \Rightarrow$$

$$\Rightarrow T_{i,m+1} - T_{i,m} \approx \lambda\left(T_{i-1,m+1} - 2T_{i,m+1} + T_{i+1,m+1}\right) - \Delta t \cdot r_{i,m+1} \Rightarrow$$

$$\Rightarrow T_{i,m} - \Delta t \cdot r_{i,m+1} \approx -\lambda \cdot T_{i-1,m+1} + (1 + 2\lambda)T_{i,m+1} - \lambda \cdot T_{i+1,m+1}$$

Operator splitting Example



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